States of Matter

Lecture 1

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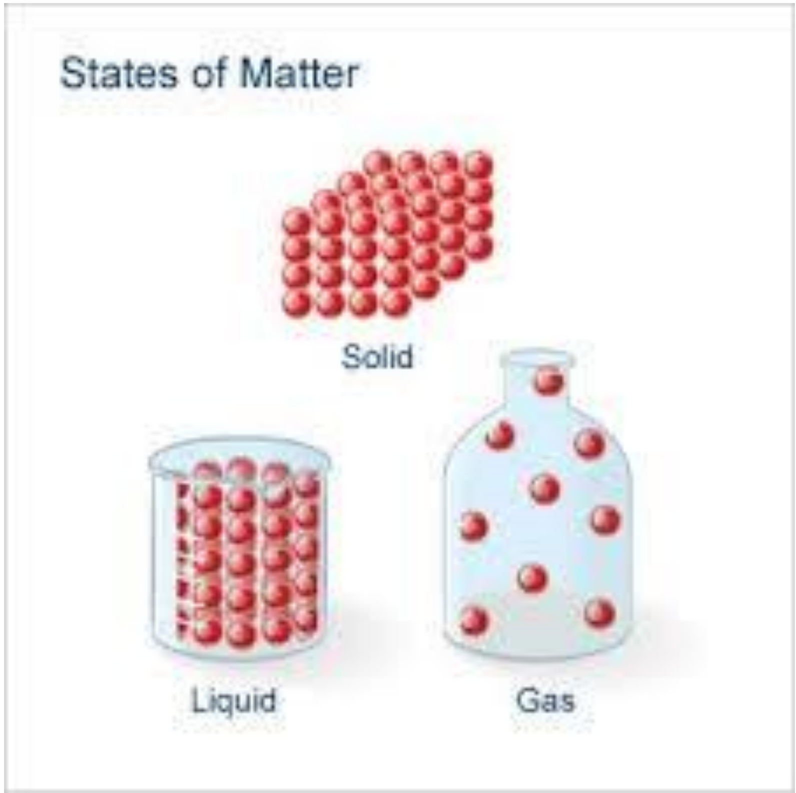
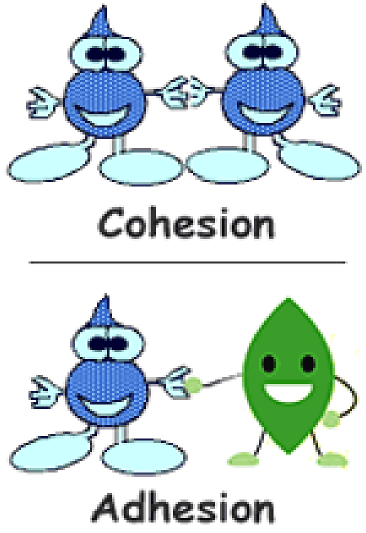
Physical pharmacy

Binding Forces Between Molecules

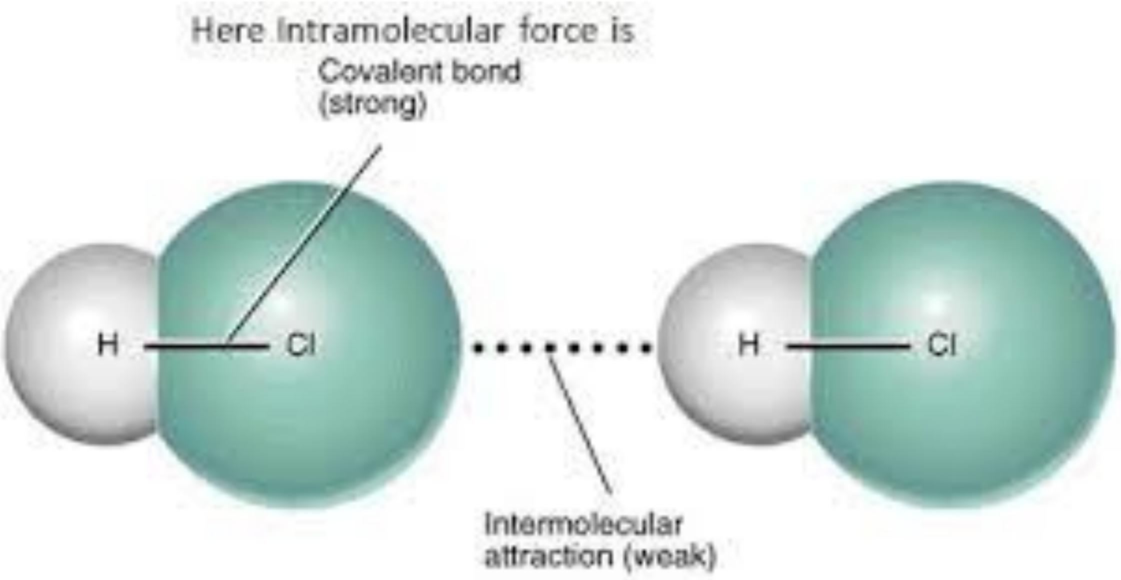
- For molecules to exist as aggregates in gases, liquids, and solids.



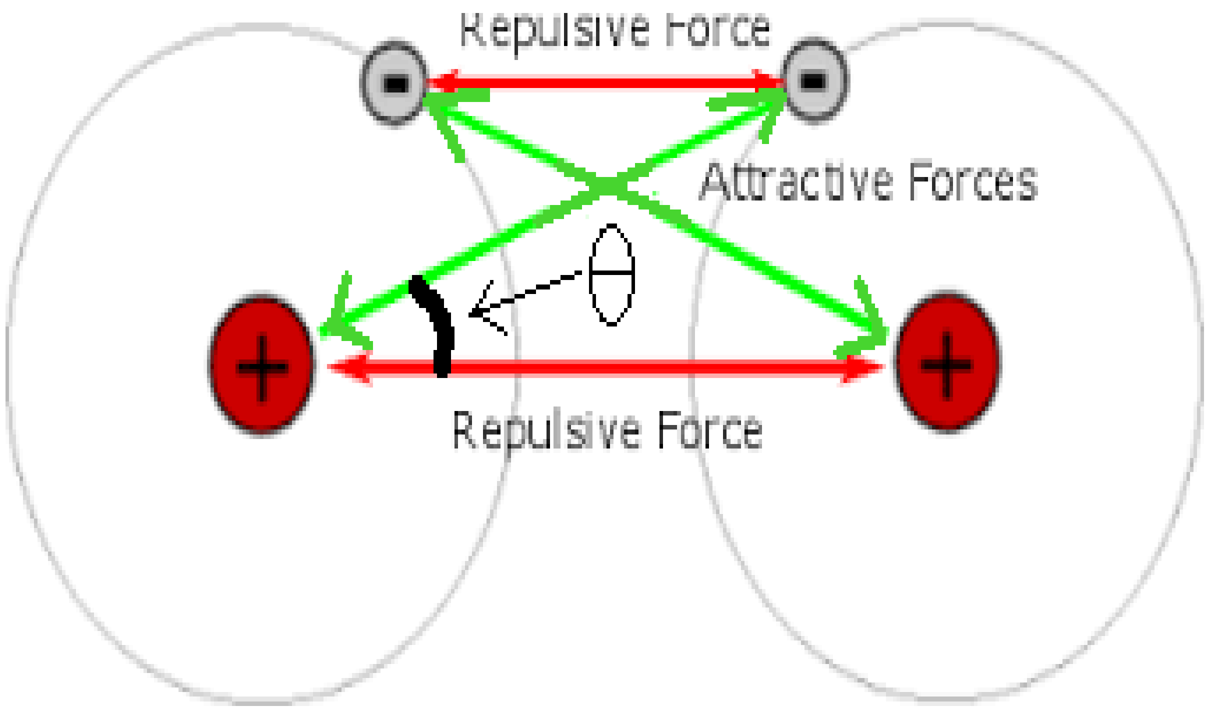
- **Intermolecular** forces must exist.
- Cohesion: the attraction of like molecules.
- adhesion: the attraction of unlike molecules are manifestations of intermolecular forces.
- Repulsion is a reaction between two molecules that forces them apart.



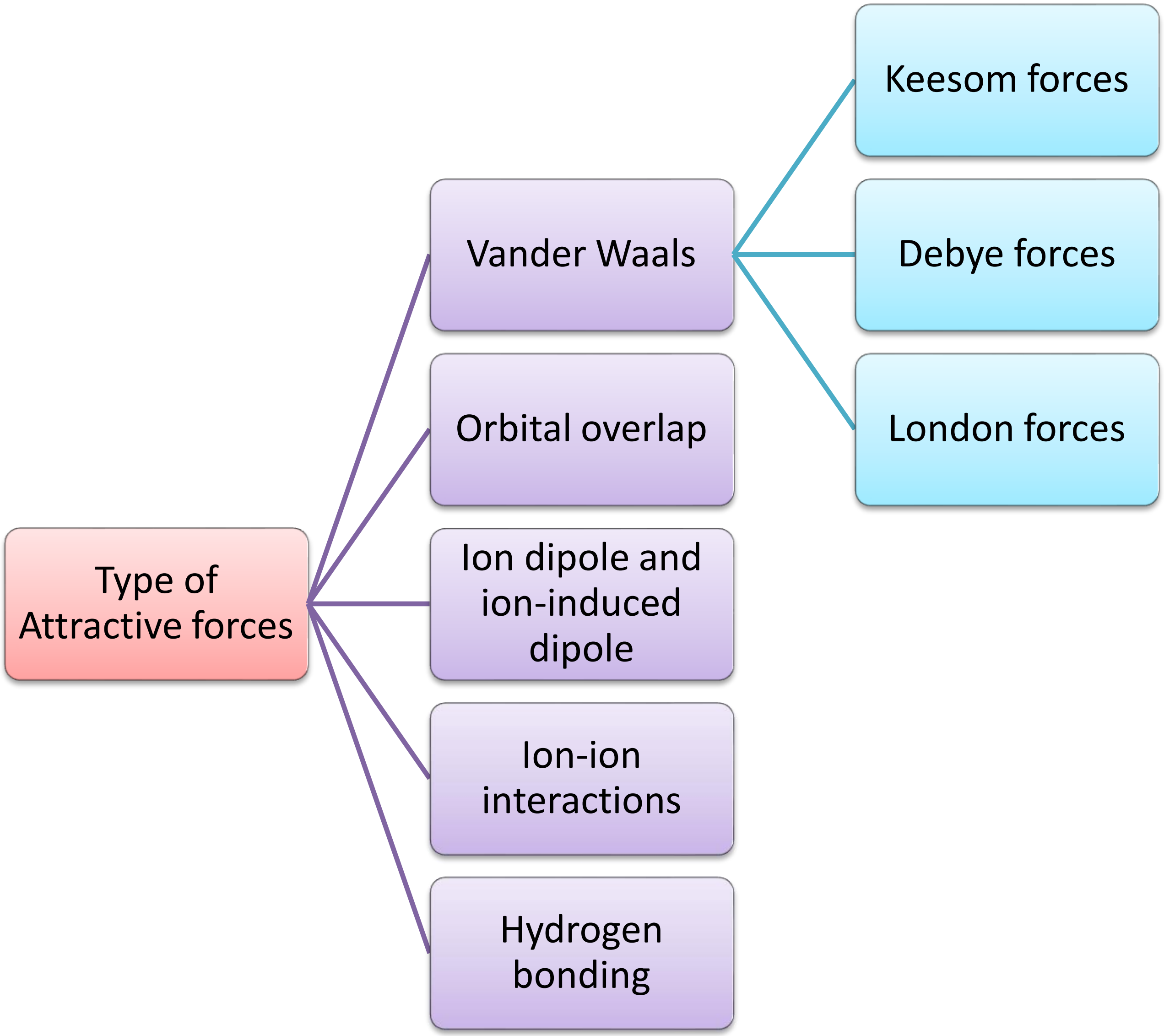
- **Intermolecular** vs **Intramolecular**



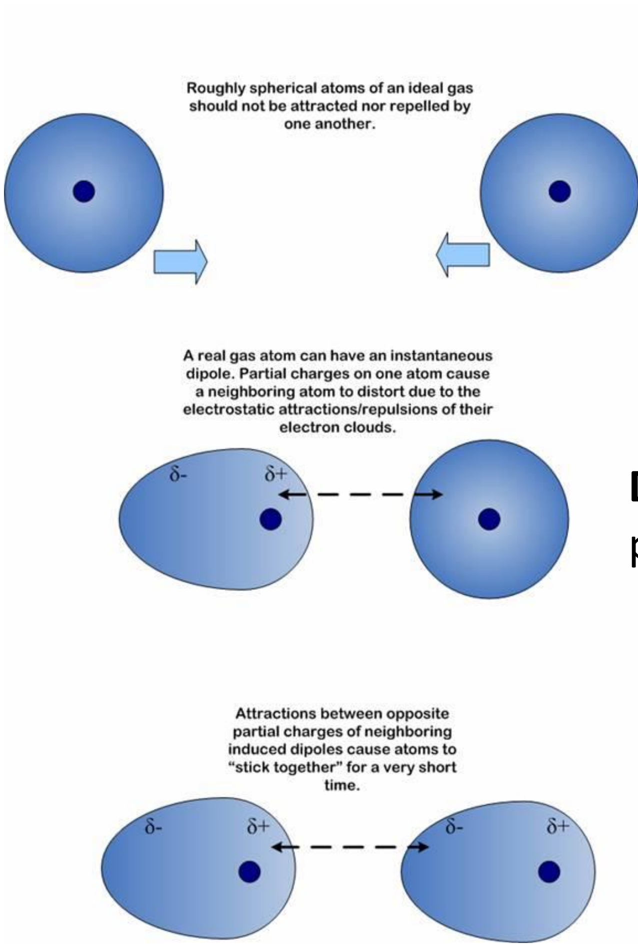
Repulsive and Attractive Forces



Attractive forces are necessary for molecules to cohere, whereas repulsive forces act to prevent the molecules from interpenetrating and annihilating each other.


Type of Attractive forces
Vander Waals
Orbital overlap
Ion dipole and ion-induced dipole
Ion-ion interactions
Hydrogen bonding
Keesom forces
Debye forces
London forces

Van der Waals Forces



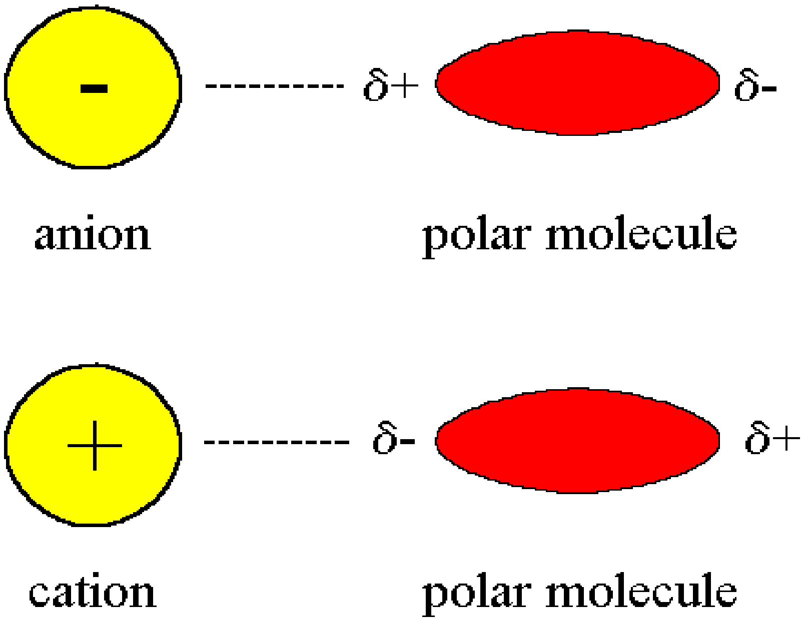
In London forces, two neighboring neutral molecules

Debye forces show the ability of a permanent dipole to polarize charge in a neighboring molecule.

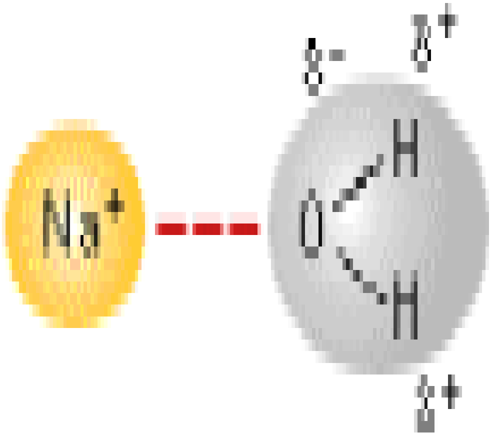
In a permanent dipole, **called keesom forces.**

Ion-Dipole and Ion-Induced Dipole Forces:

- They occur between polar or non-polar molecules and ion.
- These types of interactions account in part for the solubility of ionic **crystalline** substances in water, the cation for example attracting the relatively negative oxygen atom of water and the anion attracting the hydrogen atoms of the dipolar water molecules.



-
δ+
δ-
anion
polar molecule
+
δ-
δ+
cation
polar molecule



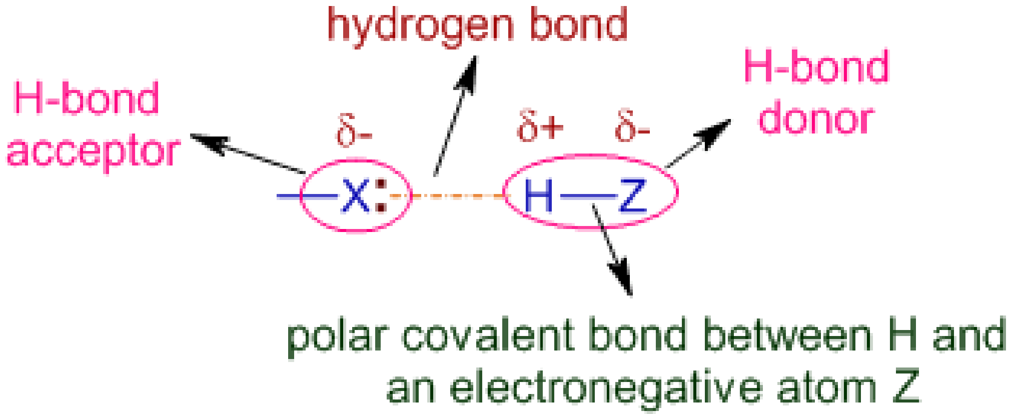
Na+
O
H
H
δ-
δ+
δ+

- Ion-induce dipole forces are involved in the formation of iodide complex and accounts for solubility of iodide in a solution of potassium iodide.

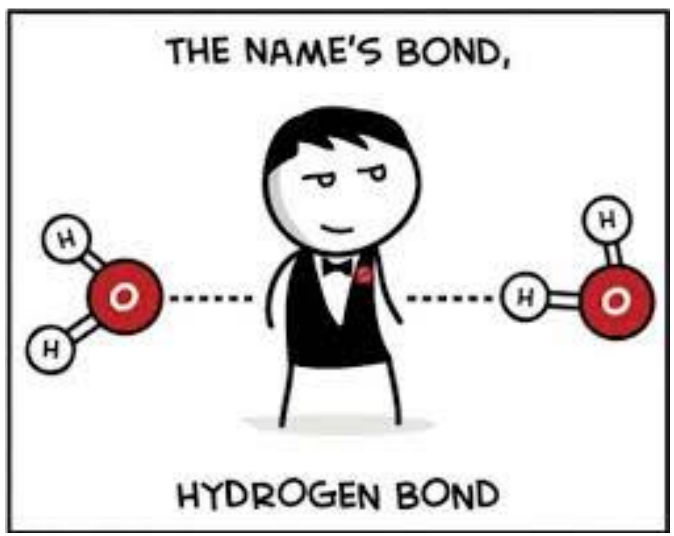
$$I_2 + K^+I^- = K^+I_3^-$$

Hydrogen Bonds

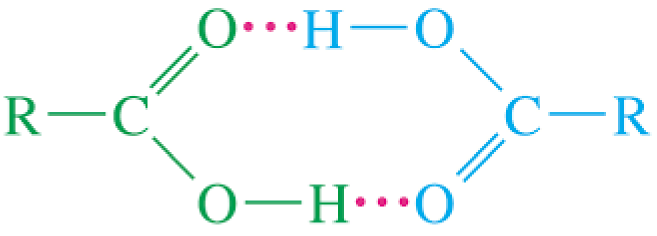
- The interaction between a molecule containing a **hydrogen atom** and a strongly electronegative atom such as **fluorine, oxygen, or nitrogen** is of particular interest.



- Such a bond, exists in ice and in liquid water; it accounts for many of the unusual properties of water including its high dielectric constant, abnormally low vapor pressure, and high boiling point.

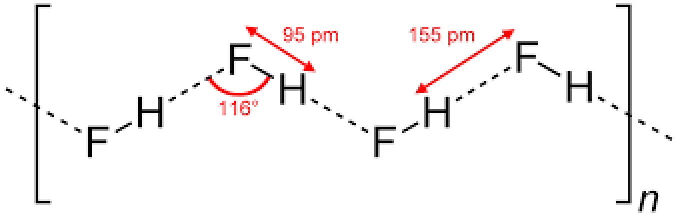


- Hydrogen bonds can also exist between alcohol molecules, carboxylic acids, aldehydes, esters, and polypeptides.
- The hydrogen bonds of formic acid and acetic acid are sufficiently strong to yield dimers (two molecules attached together), which can exist even in the vapor state.

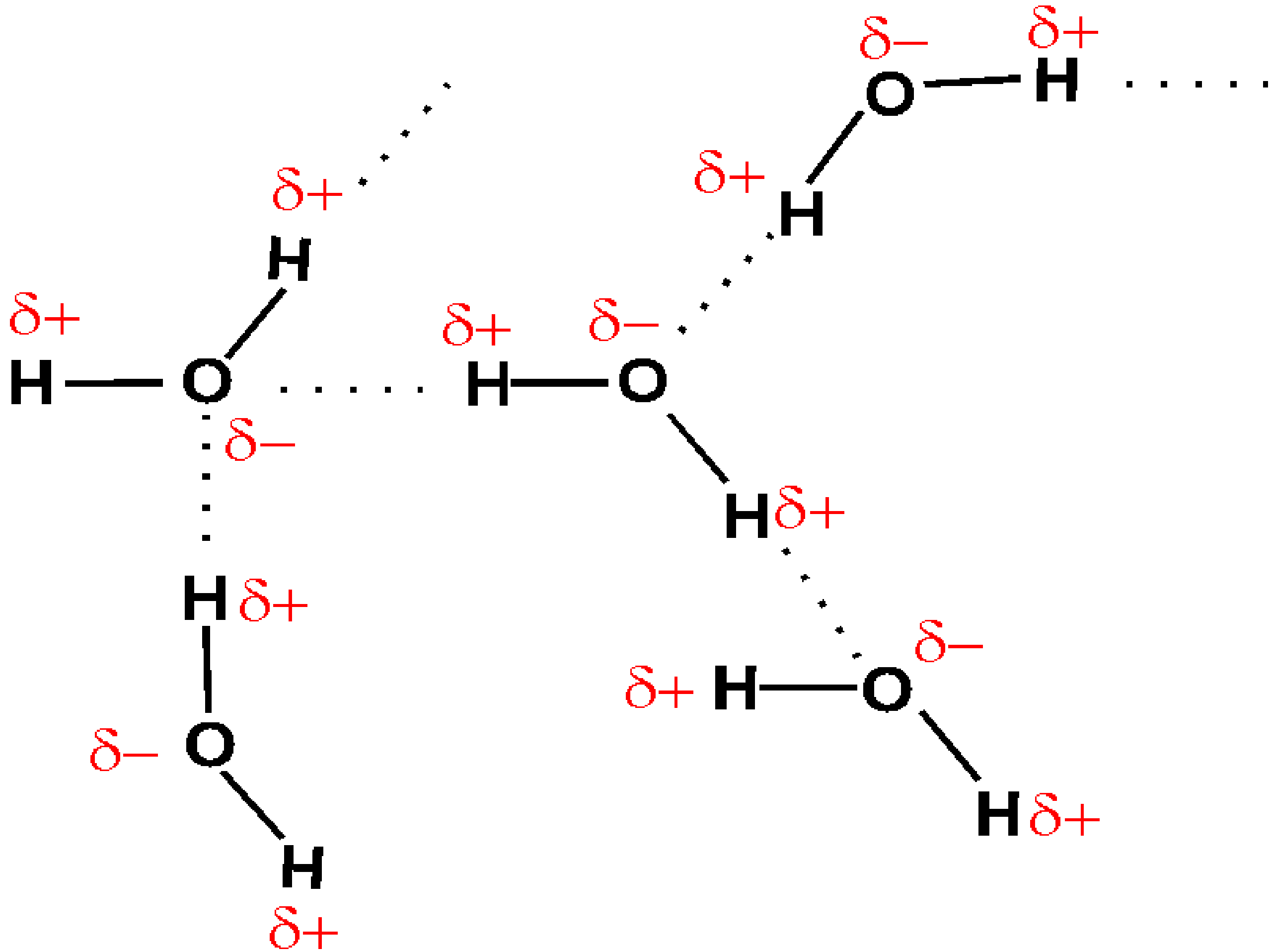


hydrogen-bonded acid dimer

- Hydrogen fluoride in the vapor state exists as a hydrogen-bonded polymer (F—H ...)n, where n can have a value as large as 6. This is largely due to the high electronegativity of the fluorine atom interacting with the positively charged hydrogen atom.

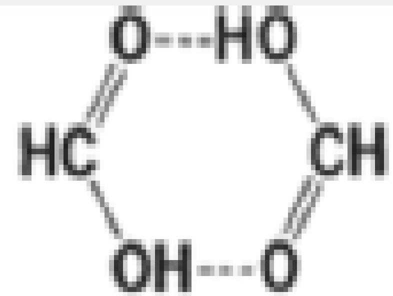


- It will be noticed that intra- as well as intermolecular hydrogen bonds may occur (as in salicylic acid).

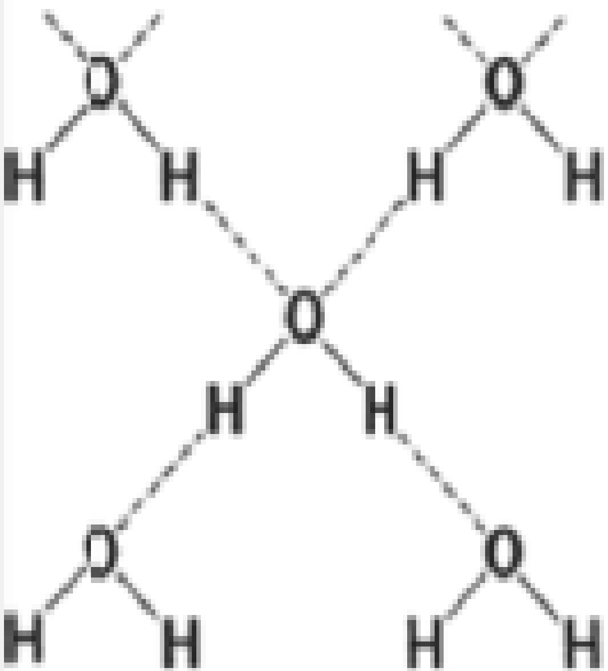


δ− δ+
H
O
δ+
H
δ+
H
δ+
H O
δ+
H O
δ− δ−
H δ+
δ−
H δ+
δ+ H O
δ−
O
H δ+
H
δ+

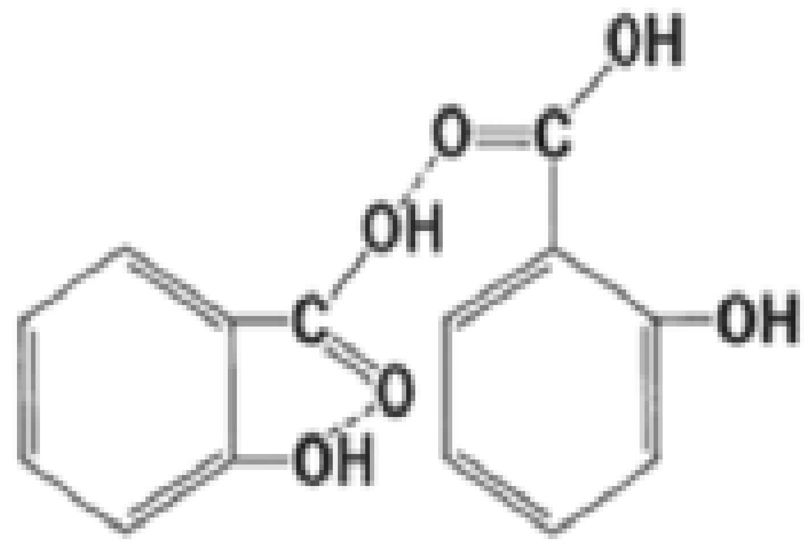
Hydrogen fluoride



Formic acid dimer



Water



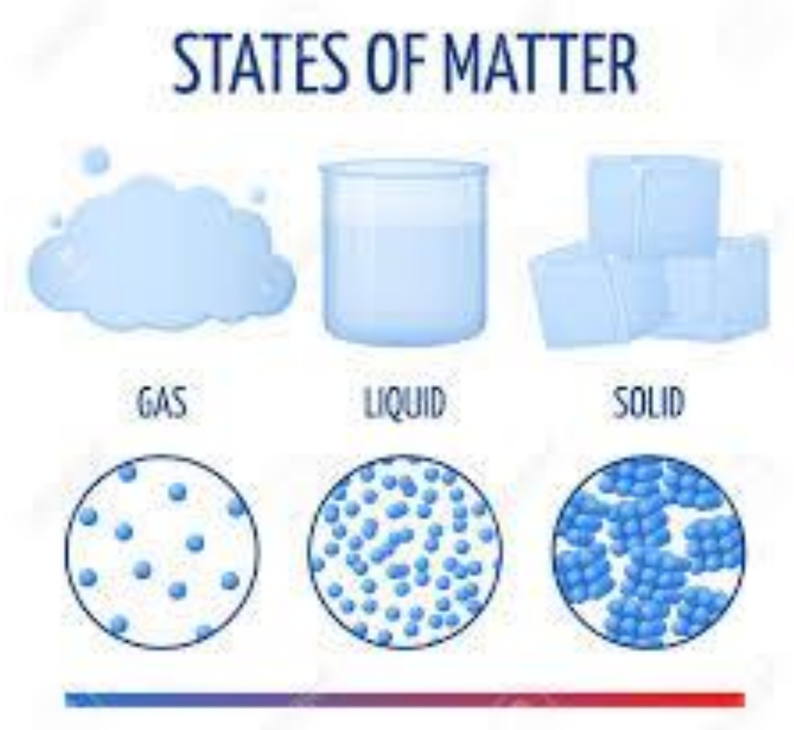
Salicylic acid showing intermolecular and intramolecular hydrogen bonding

Table 2-1 Intermolecular Forces and Valence Bonds

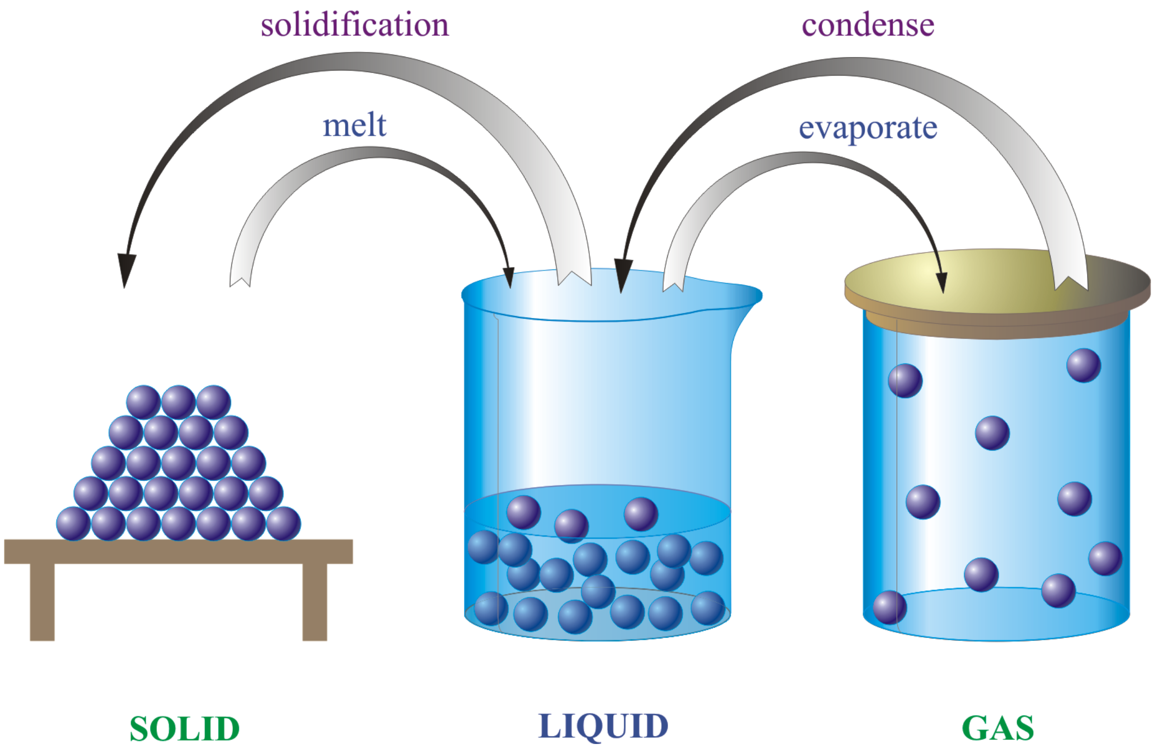
Bond Type	Bond Energy (approximately) (kcal/mole)
Van der Waals forces and other intermolecular attractions	
Dipole–dipole interaction, orientation effect, or Keesom force	
Dipole-induced dipole interaction, induction effect, or Debye force	1–10
Induced dipole–induced dipole interaction, dispersion effect, or London force	
Ion–dipole interaction	
Hydrogen bonds: O—H· · ·O	6
C—H· · ·O	2–3
O—H· · ·N	4–7
N—H· · ·O	2–3
F—H· · ·F	7
Primary valence bonds	
Electrovalent, ionic, heteropolar	100–200
Covalent, homopolar	50–150

States of Matter

- Gases , liquids and crystalline solids are the three primary states of matter .



- The molecules , atoms ,ions in the solid state are held in close proximity by intermolecular , interatomic or ionic forces.
- The atoms in the solid can oscillate only about fixed positions. As the temperature of a solid is raised, the atoms acquire sufficient energy to disrupt the ordered arrangement of lattice and pass into the liquid form.
- Finally when sufficient energy is supplied , the atoms or molecules pass into the gaseous state


solidification
melt
condense
evaporate
SOLID
LIQUID
GAS

The Gaseous State

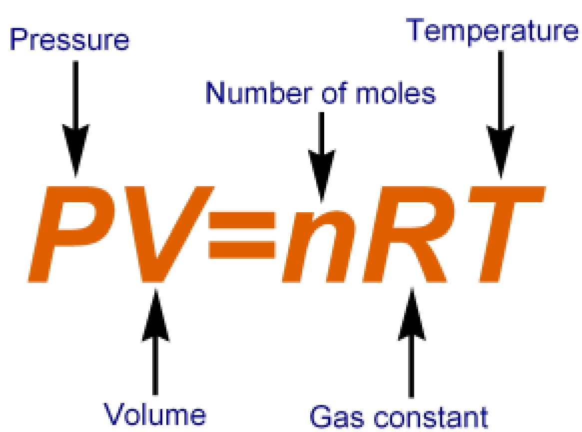
Owing to vigorous and rapid motion and resultant collisions, gas molecules travel in random paths and collide not only with one another but with the walls of containers in which they are confined. Hence, they exert a **pressure** –a force per unit area- expressed in dyne $/ \mathrm{cm}^2$. Pressure is also recorded in atmosphere or in milliliters of mercury.

Another characteristic is **volume** which is expressed in liters or cubic centimeters .

- The **temperature** is measured in absolute or kelvin scale. Zero degrees of centrigrade is equal to 273.15 K.

Ideal Gas Equation

Refer to ideal situation where no intermolecular interaction exist and no energy is exchanged upon collision.



- The conditions 0 ˚C and 1 atm are called **standard temperature and pressure (STP).**

- Experiments show that at STP, 1 mole of an ideal gas occupies 22.414 L.

$PV = nRT$

$$R = \frac{PV}{nT} = \frac{(1\ \text{atm})(22.414\text{L})}{(1\ \text{mol})(273.15\ \text{K})}$$

$$R = 0.082057\ \text{L} \bullet \text{atm} / (\text{mol} \bullet \text{K})$$

Example

- What is volume of 2 moles of ideal gas at 25 °C and 780 mmHg? (**1 atm =760 mmHg** and **R = 0.08205 L • atm / (mol • K)**

P= 780/760 = 1.026 atm

V= ?

n=2 mole

T= 25 °C+273= 298 k

$$PV = nRT$$

$$1.026\ \text{atm} \times V = 2\,\text{moles} \times \frac{0.08205\ \text{L} \bullet \text{atm}}{\text{mole.K}} \times 298\text{K}$$

V= 47.65 liter

Molecular Weight

The approximate molecular weight of a gas can be determined by use of the ideal gas law. The number of moles of gas *n* is

P.24

replaced by its equivalent *g/M*, in which *g* is the number of grams of gas and *M* is the molecular weight:

$$PV = \frac{g}{M}RT \qquad (2\text{–}7)$$

or

$$M = \frac{gRT}{PV} \qquad (2\text{–}8)$$

Example 2-3

Molecular Weight Determination by the Ideal Gas Law

If 0.30 g of ethyl alcohol in the vapor state occupies 200 mL at a pressure of 1 atm and a temperature of 100°C, what is the molecular weight of ethyl alcohol? Assume that the vapor behaves as an ideal gas. Write

$$M = \frac{0.30 \times 0.082 \times 373}{1 \times 0.2}$$

$$M = 46.0 \text{ g/mole}$$